Space Technology Research Grants

Computational Design of Nanomaterials by Pattern Replication

Completed Technology Project (2011 - 2015)

Project Introduction

Nanotechnology is a rapidly growing field with a plethora of novel applications and potential breakthroughs on the horizon. Some of the most exciting technologies that require nanometer scale features include disk drives and memory storage devices, light-emitting diodes, solar energy devices, and microarrays for genomics, proteomics, and tissue engineering applications. Along with new advances in this field comes the challenge to enable the reliable, low-cost manufacture of these technologies in order to bring this fascinating science to the general public. Currently, nanopatterning is often carried out using various lithography techniques. Despite their successes in many applications, one of the challenges facing such lithographic methods is their inability to generate patterns smaller than 20nm in a way that is reliable, cost-effective and rapid enough for industrial-scale manufacturing processes. Understanding how to overcome these engineering hurdles is the reason for my interest in self-assembly as a chemical engineering graduate student. In short, I am interested in developing strategies to induce nanometer scale particles to arrange themselves into specific patterns required for the aforementioned technological applications. There are plenty of examples that illustrate the possibilities of self-assembly, both in nature (DNA, protein folding, etc.) and through artificial means. However, it is also widely appreciated that self-assembly processes involving nanoparticles are limited in terms of the number of large-scale, low-defect structures that they can produce under various thermodynamics conditions. If the true potential of nanotechnology is to be reached, we must uncover ways to reach any desired structure. This is where "directed" self-assembly can be useful. It is possible, for example, to use traditional lithographic techniques to create a pattern on a significantly coarser lengthscale than the desired structure that helps to direct the self-assembly of particles on a finer scale (pattern multiplication). My research proposal will seek to elucidate the possibilities and limitations of this method of directed self-assembly. Specifically, the goal of this project will be to create computational tools that help discover new directed self-assembly strategies for scalable nanomanufacturing. The aim of this project is to use computational tools taken from inverse statistical mechanics to allow for a "bottom up" design of nanomaterials. Traditionally, the forward method of equilibrium statistical mechanics predicts bulk properties given knowledge about particle interactions. Conversely, the inverse methods allow an investigator to determine the particle interactions that yield desired material properties. Whit this theoretical framework, it is possible to design a material's macroscopic behavior by taking advantage of the ability to tune nanoparticle interactions (design from the bottom up). For this proposal, the focus will be on the design of materials through the use of two-dimensional patterning of nanoparticles on a substrate. With a pre-patterned substrate, it is possible to influence nanoparticles assemble into various structures. I intend to investigate the minimum amount of existing scaffolding required to allow nanoparticles to build the desired defect-free pattern (i.e., how much direction is required for directed self-assembly). In the end, I hope to create a design

Project Image Computational Design of Nanomaterials by Pattern Replication

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Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Responsible Program:

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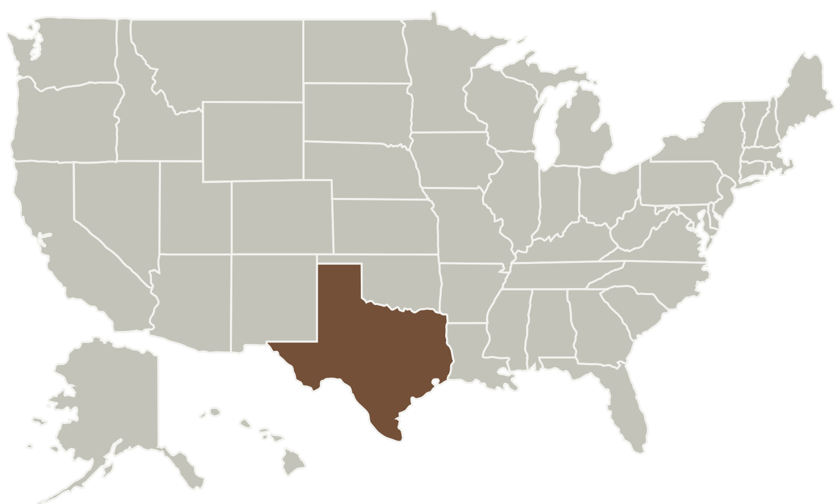
strategy for the creation the coarse length scale designs that can direct self-assembly of more detailed nanoscale patterns.

Anticipated Benefits

The aim of this project is to use computational tools taken from inverse statistical mechanics to allow for a "bottom up" design of nanomaterials. Traditionally, the forward method of equilibrium statistical mechanics predicts bulk properties given knowledge about particle interactions. Conversely, the inverse methods allow an investigator to determine the particle interactions that yield desired material properties. With this theoretical framework, it is possible to design a material's macroscopic behavior by taking advantage of the ability to tune nanoparticle interactions (design from the bottom up).

Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
The University of Texas at Austin	Supporting Organization	Academia	Austin, Texas

Primary U.S. Work Locations
Texas

Project Management

Program Director:
Claudia M Meyer

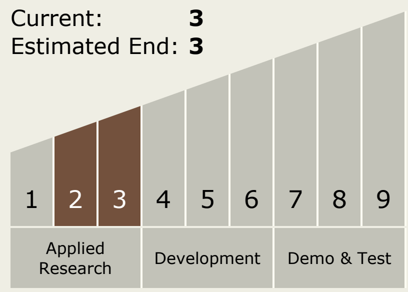
Program Manager:
Hung D Nguyen

Principal Investigator:
Thomas Truskett

Co-Investigator:
Mark E Ferraro

Technology Maturity (TRL)

Start: **2**
Current: **3**
Estimated End: **3**



Technology Areas

Primary:

- TX12 Materials, Structures, Mechanical Systems, and Manufacturing
  └ TX12.1 Materials
    └ TX12.1.2 Computational Materials

Images

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Project Image Computational Design of Nanomaterials by Pattern Replication
(https://techport.nasa.gov/image/1732)

Project Website:

https://www.nasa.gov/directorates/spacetech/home/index.html